

(1)

Ru	0.02400000	-0.04700000	-0.03500000
C	2.88946481	-0.64064142	0.15282915
C	2.77515876	0.82379006	-0.25373381
C	-1.61959472	-0.90237542	1.14601258
C	-1.76250843	-1.41940846	-0.16794365
C	-1.58398695	0.52168274	1.36223239
C	-1.73439637	-0.51779043	-1.27038437
C	-1.71711691	1.41252793	0.26174336
C	-1.76099984	0.90473219	-1.05499990
H	1.54045798	-2.25779604	-0.01019646
H	-1.51794768	-1.57997054	1.99147017
H	-1.74326169	-2.49366402	-0.33949863
H	-1.71241099	-0.90652392	-2.28640890
H	-1.73724250	1.58228500	-1.90493707
H	-1.62543009	2.48393725	0.42506538
H	-1.43921838	0.91387219	2.36612226
H	3.67631473	-1.16012005	-0.42065484
H	3.13976465	-0.73680827	1.22730326
H	3.55205075	1.44181324	0.22704301
H	2.89177072	0.91602472	-1.35146288
N	1.55470026	-1.23636046	-0.10954057
O	1.47703187	1.32737225	0.13349958

(2)

Ir	0.00000000	0.00000000	0.00000000
C	1.36805351	2.71096762	0.60200736
C	0.63109150	1.37028231	-1.43656179
C	1.61483496	2.41145606	-0.90055836
C	-0.81684930	1.49043517	-1.30804208
C	-1.49899860	2.72173958	-0.68320542
C	-0.78978541	1.42963842	1.37812447
C	-1.75742332	2.47754546	0.82450950
C	0.65499994	1.53350736	1.29299988
C	0.51044971	-3.04317047	0.01269354
C	-0.93650824	-3.05295049	-0.46047463
H	2.62910967	2.00733031	-1.03022645
H	-1.71153274	3.41940284	1.40293384
H	1.22476531	1.09480400	2.11805837
H	2.32554016	2.90020033	1.10586178
H	0.77305024	3.62782365	0.72232703
H	1.57194215	3.33592493	-1.50415338
H	-2.44762136	2.92011601	-1.20210859

H	-0.88376633	3.62183859	-0.83421355
H	-2.77813536	2.08988572	0.95890451
H	1.00436522	0.85541938	-2.32989578
H	-1.39788665	1.02232163	-2.11043776
H	-1.17364773	0.90664129	2.26267951
H	2.09164234	-1.71417650	-0.15016355
H	-2.46152250	-1.74546774	-0.21407836
H	-1.44239645	-3.99336890	-0.20000160
H	-0.98725081	-2.88719706	-1.54639519
H	0.55541235	-3.41656701	1.05281923
H	1.07475214	-3.75807487	-0.61002584
N	1.06865004	-1.67708034	-0.08320005
O	-1.60610671	-1.92883707	0.22742551

(3)

Ir	0.00000000	0.00000000	0.00000000
C	1.40763435	2.72079764	0.62717688
C	0.73583136	1.35784043	-1.41395268
C	1.70257612	2.40352230	-0.86217262
C	-0.72020522	1.50131656	-1.32993963
C	-1.40694101	2.74831243	-0.73606005
C	-0.78875648	1.47084283	1.36264147
C	-1.72219920	2.52352867	0.76419800
C	0.65499994	1.54946267	1.29299988
C	0.58250387	-3.05600635	-0.19843585
C	-0.89716835	-3.13834352	-0.58445697
C	-3.18783992	-1.37798669	-0.88161517
H	2.71785564	1.99201707	-0.95596441
H	-1.68047075	3.47149556	1.33309920
H	1.19963275	1.10157907	2.13039113
H	2.34641291	2.90390701	1.16731885
H	0.82181758	3.64609360	0.72655867
H	1.68088999	3.31775726	-1.48215151
H	-2.33200812	2.95846463	-1.29173947
H	-0.77178047	3.63680219	-0.87082400
H	-2.75374967	2.15573471	0.87042986
H	1.12285414	0.84316220	-2.30200812
H	-1.27994467	1.05193238	-2.15825825
H	-1.19254502	0.98442768	2.25688499
H	2.08803116	-1.65411800	-0.41699333
H	-1.31698737	-4.12680260	-0.36503656
H	-1.02980193	-2.90477451	-1.64800143
H	0.73131527	-3.49955787	0.80430346

H	1.13888335	-3.69553185	-0.90651010
H	-3.73618801	-0.53591035	-0.45125977
H	-3.86043571	-2.22870824	-1.03239333
H	-2.71689750	-1.07228775	-1.82009600
N	1.07781293	-1.66151399	-0.23547170
S	-1.86861320	-1.82746082	0.37168721

(4)

Ru	0.01300000	0.02300000	-0.27199997
C	-2.89426188	0.49103025	0.50050057
C	-2.75524337	-0.89962210	-0.12797649
C	1.42064949	0.53658928	1.60023170
C	1.55982606	1.43023516	0.47424730
C	1.48348794	-0.84005357	1.38495016
C	1.96503955	0.94916675	-0.80454990
C	1.71145614	-1.35256155	0.05641987
C	2.01599981	-0.46581478	-1.01299991
H	-0.52712323	-0.00402274	-1.79561804
H	-2.00007317	1.61369729	-1.02184437
H	-1.61836730	2.17670307	0.48060158
H	1.18923573	0.93241455	2.58766992
H	1.44480408	2.50343125	0.62516769
H	2.15721470	1.64049012	-1.62110737
H	2.23117106	-0.86563566	-2.00130991
H	1.67428618	-2.42431363	-0.12388068
H	1.27197019	-1.53319148	2.19691217
H	-3.86633834	0.96837433	0.29789597
H	-2.73788975	0.42566850	1.58440137
H	-3.49425151	-1.58804011	0.32389127
H	-2.99871924	-0.82244663	-1.21309643
N	-1.75946056	1.31877089	-0.06679932
O	-1.45236692	-1.39025979	0.09168528

(5)

Ir	0.00000000	0.00000000	0.00000000
C	1.48408957	2.62606802	0.60474370
C	0.71098289	1.43880568	-1.54088287
C	1.74571734	2.36513862	-0.90643330
C	-0.68694253	1.59588555	-1.42373475
C	-1.35732670	2.77298352	-0.70622221
C	-0.72927073	1.40237150	1.36643329
C	-1.66629458	2.46064717	0.78677922
C	0.73399993	1.46149178	1.28299988

C	0.65780822	-2.71065857	-1.76976598
C	-0.61020651	-2.16944010	-2.41735629
H	-0.00287044	-1.08429284	1.22977350
H	2.73288002	1.89181048	-1.02167487
H	-1.65051797	3.39253589	1.38331163
H	1.27462610	1.04469983	2.13879812
H	2.44692558	2.78479085	1.11107003
H	0.91894720	3.56144557	0.73484222
H	1.80687782	3.32301672	-1.45590006
H	-2.28878592	3.03140562	-1.23019704
H	-0.71597145	3.66297084	-0.78123396
H	-2.69209668	2.06933237	0.86637290
H	1.07620242	0.90902812	-2.42909708
H	-1.29479799	1.13675184	-2.21282085
H	-1.13266919	0.95081239	2.27897575
H	1.93074973	-1.96872143	-0.28480577
H	2.01673283	-1.11360393	-1.69688815
H	-2.09654999	-1.00900243	-1.71491546
H	-1.17361540	-2.98228666	-2.89893061
H	-0.37196427	-1.40119062	-3.16960346
H	0.38382425	-3.46341963	-1.02023591
H	1.28666922	-3.19660984	-2.53193305
N	1.37490158	-1.60329892	-1.06307082
O	-1.40156776	-1.58608934	-1.33295526

(6)

Ir	0.00000000	0.00000000	0.00000000
C	1.41908335	2.69496710	0.58921479
C	0.64126799	1.49424876	-1.54409477
C	1.68027312	2.42402545	-0.91786331
C	-0.75275295	1.63129808	-1.39481411
C	-1.43089558	2.77488147	-0.63342978
C	-0.72380976	1.38398110	1.39687749
C	-1.71130400	2.41460959	0.85289500
C	0.73399993	1.49990130	1.28299988
C	1.17065956	-2.79521311	-1.44304007
C	-0.10349300	-2.58193811	-2.26020675
C	-2.68835497	-1.22429316	-2.29254183
H	0.06151791	-1.05891936	1.24295384
H	2.66841454	1.94824146	-1.02414202
H	-1.72954200	3.33039173	1.47403881
H	1.30558249	1.10840921	2.12940498
H	2.37919718	2.92227656	1.07592781

H	0.80987748	3.60470396	0.70794925
H	1.74724844	3.37696655	-1.47660429
H	-2.37581962	3.02767607	-1.13626998
H	-0.81022574	3.67973637	-0.69416838
H	-2.71794100	1.97574487	0.92957081
H	0.98891476	0.97494242	-2.44481490
H	-1.36960227	1.17183110	-2.16745831
H	-1.08927886	0.91407288	2.31559914
H	2.28219289	-1.63596914	-0.09902710
H	2.21870516	-0.98415408	-1.61604616
H	-0.47405877	-3.53236623	-2.66157730
H	0.05856200	-1.87214016	-3.08199537
H	0.95466518	-3.44386140	-0.58437185
H	1.92958055	-3.30313043	-2.06029931
H	-3.22889954	-0.44090955	-1.75241050
H	-2.21486390	-0.79189803	-3.17945843
H	-3.35885516	-2.04251440	-2.57224042
N	1.67179079	-1.48731768	-0.90767335
S	-1.39336654	-1.83920754	-1.08063381

(7)

Ru	-0.04100000	-0.43699996	-0.19399998
C	1.36929937	0.00172630	2.36882748
C	2.40082597	0.14873021	1.25269714
C	-1.78774550	-1.66656885	-0.77749102
C	-2.23986163	-0.32616710	-0.70133792
C	-0.68115849	-2.00889642	-1.63267875
C	-1.50109162	0.69354891	-1.36782138
C	-0.03455059	-1.00642040	-2.39941474
C	-0.40299996	0.35168759	-2.23499979
C	-0.59807806	-3.80767591	2.91694058
H	-0.82938552	-1.96179603	2.19207672
H	-0.73683070	0.26012343	2.33424359
H	1.51233655	-0.94799400	2.91840902
H	1.45113519	0.82059089	3.10242908
H	3.37654979	-0.27355640	1.54589727
H	2.54837733	1.22030958	1.01503063
H	-2.25009932	-2.43073066	-0.15697115
H	-3.04836403	-0.06280314	-0.02289956
H	-1.75720259	1.73955413	-1.21266502
H	0.16967693	1.13772939	-2.72171539
H	0.84668329	-1.26060351	-2.98376660
H	-0.31787227	-3.03349668	-1.66133453

H	0.20494129	-3.97311041	2.18294130
H	-1.25485331	-4.68648200	2.92129579
H	-0.14951325	-3.70008008	3.91830802
N	0.03418351	0.01163280	1.70484021
O	1.94210598	-0.53643194	0.06382066
O	-1.41526495	-2.65934497	2.57630572

(8)

Ir	0.00000000	0.00000000	0.00000000
C	1.35508189	2.72062822	0.58012989
C	0.61668896	1.36286248	-1.45087874
C	1.59534996	2.41225140	-0.92319662
C	-0.83122672	1.47108533	-1.30576533
C	-1.52054430	2.70334297	-0.68987608
C	-0.78406155	1.43992732	1.38148816
C	-1.76345547	2.47450002	0.82269443
C	0.65499994	1.55143219	1.29299988
C	0.51259498	-3.07147851	0.01275845
C	-0.95491628	-3.13469394	-0.38985840
C	2.63491316	-1.53626337	3.77795459
H	2.61266371	2.01925144	-1.05812575
H	-1.71996660	3.42289757	1.38965547
H	1.24290081	1.10976725	2.10160827
H	2.31413399	2.91875958	1.07616035
H	0.75359629	3.63425519	0.69254851
H	1.53796210	3.33325433	-1.53068106
H	-2.47535345	2.88453603	-1.20300802
H	-0.91637596	3.60700423	-0.86040354
H	-2.77933784	2.08093188	0.97119822
H	0.98613684	0.84725182	-2.34510448
H	-1.41920669	0.98749582	-2.09334929
H	-1.16284012	0.90993352	2.26416001
H	2.05135470	-1.73298518	-0.35494219
H	-2.50582361	-1.87251598	-0.11357898
H	-1.40310249	-4.09100017	-0.08191712
H	-1.06658888	-3.00861646	-1.47676437
H	0.62219896	-3.41903966	1.05595284
H	1.06440110	-3.78356228	-0.62296971
H	2.21575479	-1.31212347	1.84068483
H	2.50168253	-2.62303976	3.91071616
H	1.71328392	-1.02438472	4.09775814
H	3.45482302	-1.20318987	4.42505688
N	1.05026803	-1.69528568	-0.13160897

O	-1.63836756	-2.03512073	0.31258759
O	3.00878163	-1.20021183	2.41970691

(9)

Ir	0.00000000	0.00000000	0.00000000
C	1.42731940	2.71491616	0.61586386
C	0.78614745	1.32608032	-1.41578178
C	1.74669163	2.37823409	-0.86313836
C	-0.67557897	1.46819531	-1.36037158
C	-1.37162104	2.72860165	-0.80808909
C	-0.78883422	1.50785705	1.34255429
C	-1.69742020	2.55588038	0.69746288
C	0.65499994	1.56602431	1.29299988
C	0.65252941	-3.03904526	-0.34858225
C	-0.83583854	-3.13612001	-0.66874669
C	2.87695308	-1.50592292	3.47483367
C	-3.22736798	-1.63122125	-0.77924054
H	2.76356092	1.96680628	-0.93014575
H	-1.64380883	3.52257991	1.23178142
H	1.18737402	1.10695915	2.13078470
H	2.35992413	2.90137919	1.16493265
H	0.84470132	3.64466387	0.69018225
H	1.74290560	3.28782634	-1.49124587
H	-2.29486463	2.91437844	-1.37503370
H	-0.73777300	3.61338988	-0.97140733
H	-2.73524885	2.20980311	0.80840417
H	1.18639660	0.80044311	-2.29135201
H	-1.22036354	1.00450043	-2.19023651
H	-1.21869380	1.04169921	2.23480289
H	2.04331445	-1.56911931	-0.80930601
H	-1.23982184	-4.13702707	-0.47777934
H	-1.02759789	-2.84845662	-1.70900260
H	0.84893362	-3.49859779	0.63584763
H	1.19942413	-3.64262166	-1.09196472
H	2.42803674	-1.45771648	1.52152357
H	2.40261398	-2.43938112	3.82590355
H	2.20151850	-0.66021060	3.68325669
H	3.80707865	-1.35161762	4.03727585
H	-3.72432335	-2.60163700	-0.89354204
H	-3.90562984	-0.90270348	-0.33026868
H	-2.87007572	-1.26151276	-1.74487698
N	1.11382620	-1.62711558	-0.37708331
O	3.24012114	-1.58351650	2.07157436

S	-1.78464457	-1.88823645	0.39651208
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(10)

Ru	-0.01300000	0.08499999	-0.14699999
C	1.29181439	-0.17660341	2.51350460
C	2.31483267	-0.61400513	1.46704343
C	-1.60680305	1.58392835	-0.05301595
C	-2.14963365	0.52933127	-0.83495728
C	-0.35584324	2.19472230	-0.41309429
C	-1.39217035	0.02151161	-1.92709706
C	0.34563446	1.71650904	-1.56467090
C	-0.16799998	0.63716437	-2.32899978
C	-1.12172141	-3.16281958	-0.14853919
H	-0.77721099	0.02692996	2.44944739
H	-2.12064729	1.90831243	0.85062109
H	-3.07534816	0.04557051	-0.53309412
H	-1.74407965	-0.86259404	-2.45577925
H	0.40352085	0.22887787	-3.15842493
H	1.33702264	2.10807619	-1.78432008
H	0.06701932	2.98736079	0.19996717
H	1.40941434	-0.75212820	3.44908988
H	1.43436427	0.89272603	2.75664348
H	3.33365431	-0.29083050	1.74022452
H	2.31475797	-1.71713703	1.38456404
H	-0.13111461	-1.89044581	1.13891069
H	-2.08655669	-2.69706555	0.10755555
H	-1.03022302	-4.12041688	0.38633825
H	-1.09305989	-3.35669897	-1.22716392
N	-0.03952893	-0.42397211	1.89396771
O	1.97137565	-0.00864397	0.21021684
O	-0.00238758	-2.30816798	0.18969267

(11)

Ir	0.00000000	0.00000000	0.00000000
C	1.50472106	2.69056138	0.51676118
C	0.82137164	1.23052519	-1.47732038
C	1.82468822	2.24794798	-0.93995432
C	-0.60908954	1.39972608	-1.45452467
C	-1.29809125	2.66414029	-0.90891586
C	-0.69312956	1.55654168	1.31352451
C	-1.62342433	2.53982429	0.60511269
C	0.73399993	1.60558623	1.28299988
C	-0.90701469	-2.71872490	-1.24333158

C	-2.32215017	-2.23310896	-1.59757427
C	-0.25304704	-1.75963379	2.94621874
H	2.81733974	1.77575755	-0.96198524
H	-1.60908383	3.53365072	1.08882136
H	1.26370105	1.19685055	2.14893444
H	2.44614518	2.92928237	1.03091128
H	0.92488806	3.62455883	0.51466118
H	1.88811232	3.12430835	-1.61061317
H	-2.22455374	2.84562287	-1.47163202
H	-0.65981290	3.54091367	-1.09154864
H	-2.64899958	2.16057392	0.72262776
H	1.23067362	0.62853188	-2.29853962
H	-1.16200029	0.90347213	-2.25895175
H	-1.14742845	1.10408541	2.20303903
H	0.47183620	-2.34044812	1.11043977
H	0.44987826	-1.47675992	-2.13638991
H	-3.38379738	-0.78348434	-0.69820159
H	-2.96699919	-3.08721646	-1.87110540
H	-2.28265154	-1.53077730	-2.44371331
H	-0.99596688	-3.24529562	-0.27788215
H	-0.60856520	-3.48302192	-1.98283905
H	0.00354718	-2.78361146	3.24143341
H	0.37689318	-1.04155272	3.48534392
H	-1.31414362	-1.58151310	3.14908271
N	0.13385385	-1.66834798	-1.17631211
O	-2.88686553	-1.57993930	-0.41766496
O	-0.04745152	-1.60594321	1.50520892

(12)

Ir	0.00000000	0.00000000	0.00000000
C	1.66019378	2.57639493	0.53570904
C	1.04178291	1.08014264	-1.44732511
C	2.08545761	2.01889942	-0.85205308
C	-0.36972295	1.36415035	-1.56194433
C	-1.00337673	2.70019751	-1.13463449
C	-0.69131407	1.64951045	1.17451439
C	-1.47334121	2.66802596	0.34608413
C	0.73399993	1.60590590	1.28299988
C	-0.90736709	-2.78727725	-1.06973431
C	-2.37994117	-2.49744473	-1.45669924
C	0.42626295	-1.52293781	3.04076138
C	-4.43303180	-0.48887493	-1.01989295
H	3.01742131	1.44511240	-0.74355758

H	-1.41606274	3.67700330	0.79326701
H	1.14367492	1.22604679	2.22313097
H	2.55811015	2.76706056	1.13980458
H	1.16484771	3.55119180	0.41691013
H	2.31037213	2.84223403	-1.55419934
H	-1.85853335	2.92037142	-1.78846350
H	-0.28554778	3.51833417	-1.29365583
H	-2.53296167	2.37775413	0.38103033
H	1.46132608	0.39947711	-2.19816179
H	-0.88329140	0.87577436	-2.39641618
H	-1.25401219	1.27185198	2.03707919
H	0.85886199	-2.14826763	1.15507544
H	0.23810133	-1.49015373	-2.16321076
H	-2.91657506	-3.43214022	-1.66829553
H	-2.42708242	-1.84979269	-2.34049846
H	-0.89850239	-3.19372189	-0.04757166
H	-0.56004111	-3.60761982	-1.72568886
H	0.52197006	-2.53018023	3.46778236
H	1.33265565	-0.92906184	3.22602235
H	-0.44178290	-1.02253607	3.48170655
H	-3.84532353	0.17530260	-1.66167811
H	-5.14758291	-1.06851368	-1.61564180
H	-4.97727366	0.10847505	-0.28007043
N	0.03251448	-1.65887462	-1.16900008
O	0.14477452	-1.63816084	1.60345345
S	-3.29661381	-1.61874542	-0.05769138

(13)

Ru	0.29599997	-0.20299998	-0.10999999
C	-1.05047967	0.72695521	2.45719152
C	-1.21383635	-0.79092957	2.30935443
C	2.52740694	0.73071165	-0.24798340
C	1.59630706	1.20575149	-1.24567783
C	2.66274976	-0.64000899	-0.03967453
C	0.98649323	0.30704259	-2.16717400
C	1.89125816	-1.56454611	-0.83508834
C	1.12599990	-1.09986915	-1.93799982
C	-3.94723624	0.59999682	-0.80077996
H	-1.17507331	-0.62628638	-0.61512081
H	-1.75738388	1.42484273	0.61238038
H	-0.37903696	2.19098339	1.10326601
H	3.05538587	1.44187514	0.38619313
H	1.43992518	2.27775029	-1.36514190

H	0.37182015	0.68127968	-2.98237014
H	0.60050512	-1.81220613	-2.57076870
H	1.93113185	-2.62956076	-0.61674198
H	3.28044367	-1.01563879	0.77438638
H	-1.91309460	1.21278026	2.94023179
H	-0.14372842	0.94090796	3.03804489
H	-1.24066282	-1.26164625	3.31105679
H	-2.19410888	-1.00131291	1.82309760
H	-4.93687086	0.49247069	-1.29726033
H	-3.20529846	-0.21387969	-0.95753872
N	-0.83965950	1.27360635	1.06172242
O	-0.13139766	-1.31252453	1.57061923
O	-3.68766960	1.57757581	-0.11157701

(14)

Ir	0.00000000	0.00000000	0.00000000
C	1.49995471	2.61465686	0.61181366
C	0.70968058	1.44369400	-1.53660414
C	1.75046700	2.36323949	-0.90260496
C	-0.68695665	1.60456584	-1.41396846
C	-1.35013929	2.78422752	-0.69330288
C	-0.72777296	1.40570830	1.36961371
C	-1.66123438	2.46939565	0.79698799
C	0.73399993	1.45657489	1.28299988
C	0.63791771	-2.71419156	-1.74934645
C	-0.63698098	-2.21397892	-2.41635573
C	1.63899489	-3.43198204	2.09563439
H	-0.01202849	-1.08277762	1.23149750
H	2.73419693	1.88461445	-1.02363889
H	-1.64377457	3.39945464	1.39659535
H	1.27317564	1.03226719	2.13602519
H	2.47004489	2.74815727	1.11204239
H	0.95586609	3.56135017	0.75487443
H	1.81524831	3.32371907	-1.44669937
H	-2.28129242	3.04782954	-1.21559659
H	-0.70429878	3.67168644	-0.76500485
H	-2.68813242	2.08074125	0.87398433
H	1.06940493	0.91554703	-2.42731981
H	-1.29975193	1.14731195	-2.19995695
H	-1.13112833	0.95551951	2.28273678
H	1.91689720	-1.97811561	-0.28160788
H	1.98920072	-1.11486360	-1.69718224
H	-2.13474552	-1.04323180	-1.75867606

H	-1.18217146	-3.05661050	-2.86956539
H	-0.41444901	-1.47188895	-3.19863577
H	0.36961424	-3.45497442	-0.98578929
H	1.27233204	-3.21374623	-2.49824771
H	0.63752937	-2.95553975	2.02087695
H	1.78704549	-4.20435398	2.88567643
N	1.35179680	-1.59860006	-1.05481310
O	-1.44094878	-1.60663921	-1.35604326
O	2.54848824	-3.11853036	1.34131880

(15)

Ir	0.00000000	0.00000000	0.00000000
C	1.38926723	2.70123411	0.56993792
C	0.49030877	1.51717351	-1.55013215
C	1.51199051	2.49906801	-0.97094226
C	-0.90396375	1.57267839	-1.32687035
C	-1.57508802	2.69832013	-0.52926864
C	-0.71440645	1.33728067	1.45298736
C	-1.76177429	2.33570419	0.96870016
C	0.73399993	1.50117672	1.28299988
C	1.39850427	-2.67723513	-1.49089955
C	0.05030551	-2.59986914	-2.19484698
C	1.88521552	-3.52521588	2.19876731
C	-2.70909277	-1.86204083	-2.03523044
H	0.16394396	-1.03794780	1.25354380
H	2.51143577	2.09086760	-1.18785880
H	-1.77373556	3.25240811	1.58895875
H	1.34973696	1.09864863	2.09223888
H	2.40497112	2.81846572	0.97405534
H	0.86566353	3.64271645	0.80242602
H	1.47199147	3.47372422	-1.49256085
H	-2.55201990	2.92866730	-0.97875326
H	-0.97778942	3.61725844	-0.62265876
H	-2.74728956	1.86432549	1.10439726
H	0.82253898	1.02890444	-2.47336743
H	-1.53936315	1.09369543	-2.07519731
H	-1.02312840	0.83768162	2.37678170
H	2.33654834	-1.51756414	-0.04406099
H	2.31258007	-0.79230863	-1.54057931
H	-0.23828488	-3.57290228	-2.61014167
H	0.04831692	-1.84263958	-2.98922740
H	1.34842754	-3.41619039	-0.68339472
H	2.16891862	-3.02398390	-2.19803590

H	0.82125230	-3.20951609	2.14180510
H	2.11407812	-4.45059715	2.77516047
H	-3.25404574	-2.81034716	-2.06428282
H	-2.34327025	-1.59813816	-3.03171063
H	-3.33456180	-1.06102326	-1.63409745
N	1.76585411	-1.35832203	-0.88346820
O	2.77064672	-2.88578044	1.65278626
S	-1.22828057	-2.05714920	-0.89542452

(16)-(TS)

Ru	0.29599997	-0.20299998	-0.10999999
C	-1.08592380	0.92467997	2.27744918
C	-1.28172922	-0.58823428	2.30922483
C	2.30357051	0.67537923	-0.20932481
C	1.60234881	1.10413046	-1.38371033
C	2.41795342	-0.71651751	0.08008383
C	1.00688453	0.14560828	-2.23954462
C	1.84788618	-1.68739075	-0.80409226
C	1.12599990	-1.25112770	-1.93799982
C	-2.71449360	-0.20020652	-0.99805908
H	-1.59733996	-0.54280307	-0.73154433
H	-1.92744097	1.24577247	0.28162339
H	-0.49973245	2.23718616	0.75693576
H	2.72259347	1.40821094	0.47754959
H	1.47269251	2.16586944	-1.58419796
H	0.41553296	0.46868439	-3.09276159
H	0.61226501	-1.97866846	-2.56314977
H	1.88010757	-2.74292878	-0.54646440
H	2.88350711	-1.03916938	1.00865808
H	-1.96306921	1.46061297	2.67309225
H	-0.19802311	1.21200286	2.86146169
H	-1.25419455	-0.96939422	3.34456681
H	-2.26839196	-0.83827145	1.87909015
H	-3.29271223	-1.10562203	-0.71653178
H	-2.67127444	-0.11193289	-2.10512673
N	-0.86351661	1.27800849	0.83138535
O	-0.21861373	-1.20567575	1.56732859
O	-3.05117250	0.93398556	-0.33907190

(17)-(TS)

Ir	0.00000000	0.00000000	0.00000000
C	1.51416489	2.60695449	0.58645759
C	0.75151901	1.32286755	-1.48556816

C	1.79195885	2.28025015	-0.90378304
C	-0.67368438	1.49785381	-1.36552041
C	-1.32308975	2.74205453	-0.74109746
C	-0.72146307	1.45575430	1.37308281
C	-1.64698249	2.50838711	0.75812515
C	0.73399993	1.48202953	1.28299988
C	0.33969659	-2.70832313	-1.64839059
C	-0.89644786	-2.16096311	-2.35133262
C	0.94752163	-2.03152513	2.04998493
H	0.25563854	-1.21243454	1.46034715
H	2.77568552	1.79741756	-0.98981798
H	-1.61756849	3.46381983	1.31237255
H	1.27285721	1.03276901	2.12306986
H	2.46824317	2.76548387	1.10684671
H	0.95756813	3.55138432	0.67266941
H	1.85526487	3.20629699	-1.50410500
H	-2.23720721	2.99425622	-1.29631709
H	-0.65147627	3.60379720	-0.86245664
H	-2.67721854	2.13526323	0.84997768
H	1.10729280	0.78099244	-2.36884744
H	-1.27040263	1.03237330	-2.15825629
H	-1.12798969	1.01122882	2.28878221
H	1.62240215	-2.14948272	0.11684866
H	1.84886501	-1.29593899	-1.51855689
H	-2.36870688	-0.94236729	-1.71279649
H	-1.46795813	-2.96888489	-2.83300407
H	-0.62379190	-1.40802486	-3.10694547
H	0.02216139	-3.46489103	-0.91447016
H	0.98257061	-3.21777607	-2.38184641
H	0.17163169	-2.76661730	2.35530875
H	1.27096015	-1.43304963	2.92428111
N	1.09071249	-1.64301533	-0.91810572
O	-1.71130914	-1.54058406	-1.29888698
O	1.94087758	-2.50504473	1.26713723

(18)-(TS)

Ir	0.00000000	0.00000000	0.00000000
C	1.53235211	2.63052953	0.56693248
C	0.77758334	1.29708778	-1.48784227
C	1.81068570	2.26045356	-0.91678239
C	-0.64166156	1.50567294	-1.39341550
C	-1.26723886	2.77041531	-0.78609911
C	-0.71367687	1.50213912	1.35045329

C	-1.60813367	2.56510744	0.71313050
C	0.73402162	1.52187594	1.28299000
C	0.35171717	-2.79503739	-1.56510163
C	-0.92305177	-2.43745379	-2.32392898
C	0.98441842	-2.01146780	2.02810375
C	-3.42463479	-0.93131818	-2.23787930
H	0.25457040	-1.20008658	1.45583589
H	2.79240808	1.77295200	-0.98845675
H	-1.55508993	3.52368701	1.26036354
H	1.26684366	1.08420232	2.13145498
H	2.48975612	2.76976199	1.08670355
H	1.01485203	3.59742613	0.63893267
H	1.86659190	3.16668533	-1.54683313
H	-2.17600942	3.03057412	-1.34650825
H	-0.57950428	3.61804187	-0.91676970
H	-2.64944201	2.22347198	0.79865204
H	1.13426236	0.74280291	-2.36357735
H	-1.24816255	1.04198367	-2.17328342
H	-1.13965847	1.07638331	2.26536243
H	1.62400919	-2.11129099	0.08200392
H	1.78777257	-1.30431010	-1.56215847
H	-1.37124772	-3.34645023	-2.74663347
H	-0.72320032	-1.71188229	-3.12258720
H	0.11179749	-3.52436904	-0.77618909
H	1.03359477	-3.30365135	-2.26581415
H	0.22652705	-2.76104226	2.34253850
H	1.31222899	-1.39983541	2.89096553
H	-3.84226234	-0.07430165	-1.70121353
H	-4.21026189	-1.67240981	-2.41363319
H	-3.00199384	-0.59641614	-3.19018119
N	1.05708910	-1.64575569	-0.92536738
O	1.97218852	-2.47330036	1.23825503
S	-2.12427207	-1.66513406	-1.10522956

(19)-(TS)

Ru	-0.01344500	0.08476799	-0.14651399
C	1.41870180	0.13380493	2.49362567
C	2.38774756	-0.44129698	1.45652871
C	-1.51036310	1.68112275	-0.19691653
C	-2.13775591	0.57073873	-0.83061166
C	-0.25342319	2.19126028	-0.67302223
C	-1.43238890	-0.11805759	-1.85634031
C	0.40210577	1.51922917	-1.74500162

C	-0.16763798	0.35469916	-2.32911978
C	-1.21104740	-2.92525704	0.28793069
H	-0.66804258	0.30166339	2.53176008
H	-1.98206778	2.14546178	0.66840279
H	-3.08246114	0.18525771	-0.45470012
H	-1.84245433	-1.04267820	-2.26019202
H	0.36824997	-0.19435035	-3.09973868
H	1.41092810	1.81806864	-2.02304081
H	0.22556241	3.03205690	-0.17682273
H	1.58001185	-0.31772432	3.48972916
H	1.56947468	1.22500115	2.58292411
H	3.41967387	-0.09749197	1.64581756
H	2.37864103	-1.54722770	1.51665636
H	-0.10032938	-1.48047597	1.48124583
H	-2.15213208	-2.41364378	0.55403060
H	-1.11909391	-3.83842815	0.89772530
H	-1.25386772	-3.21949859	-0.77014090
N	0.05622544	-0.17626376	1.98286263
O	1.99544547	0.01166336	0.15462982
O	-0.05906992	-2.08697921	0.50722273

(20)-(TS)

Ir	0.00000000	0.00000000	0.00000000
C	1.66432322	2.56158505	0.55060786
C	1.03412931	1.08910843	-1.44625168
C	2.07586167	2.03435524	-0.85372598
C	-0.37713899	1.38526183	-1.54865478
C	-0.99157263	2.72751020	-1.11343553
C	-0.68620575	1.65293019	1.18945431
C	-1.45403783	2.68984441	0.37058627
C	0.73399993	1.58389083	1.28299988
C	-0.95909349	-2.77769722	-1.30245628
C	-2.30939378	-2.16658803	-1.70433146
C	1.32353981	-2.02268946	2.37751076
C	-4.01779800	0.05333607	-1.01978075
H	3.02033119	1.47797039	-0.77206691
H	-1.37630692	3.69356389	0.82486662
H	1.14641261	1.15343912	2.19964145
H	2.56671789	2.72786027	1.15452436
H	1.17605157	3.54232068	0.45816766
H	2.27216594	2.87676987	-1.54189774
H	-1.84779117	2.96362237	-1.76121008
H	-0.26988637	3.54242870	-1.27107815

H	-2.51875428	2.42227595	0.40986587
H	1.44822029	0.42715944	-2.21757962
H	-0.89637790	0.91357586	-2.38982341
H	-1.25068791	1.24999723	2.03729310
H	0.51150957	-2.14094900	0.47935625
H	0.73321089	-1.76242374	-1.91593249
H	-3.00297385	-2.94218938	-2.05691040
H	-2.18531137	-1.40615788	-2.48438783
H	-1.12700466	-3.37713300	-0.39152333
H	-0.65520138	-3.49603948	-2.08182107
H	1.39796373	-3.11213810	2.49932314
H	2.28561593	-1.61564685	2.03636500
H	1.04609639	-1.56490141	3.33309901
H	-3.31706905	0.75612519	-1.48015064
H	-4.71759967	-0.33734397	-1.76610527
H	-4.58192793	0.55644441	-0.22769189
N	0.15671630	-1.81836578	-1.06973348
O	0.26040610	-1.74814658	1.42098893
S	-3.08339075	-1.33372397	-0.20008064

(21)

Ru	-0.13562499	-0.04615400	-0.05810299
C	2.60273663	-1.33632750	-0.26396435
C	2.64922264	-0.25572569	0.82183726
C	-1.55965480	-1.66098629	0.64623582
C	-1.73931552	-1.39845952	-0.75233572
C	-1.57870319	-0.56218964	1.54135512
C	-2.09774930	-0.10046355	-1.22925851
C	-1.86052886	0.76197441	1.08073120
C	-2.11210780	0.97731546	-0.31003797
C	1.02821724	2.75645601	-0.21190992
H	1.76365587	-0.05716399	-1.70195406
H	1.28432473	-1.66652721	-1.88654965
H	-1.31551188	-2.66043815	0.99730631
H	-1.62339415	-2.21391790	-1.46634129
H	-2.24802652	0.08192885	-2.29031901
H	-2.24890777	1.99233657	-0.67806179
H	-1.82737278	1.60254065	1.76910907
H	-1.29915955	-0.71389187	2.58258174
H	3.56114004	-1.43851673	-0.79767733
H	2.32759542	-2.30623878	0.17024274
H	3.32222003	-0.57235235	1.63903597
H	3.06913897	0.67234217	0.38495676

H	1.70539702	3.42669551	-0.77298176
H	0.07366528	3.30296108	-0.05981327
H	1.47515475	2.57955761	0.78484857
N	1.50054525	-0.92936186	-1.20629898
O	1.34876305	-0.05232397	1.35458514
O	0.85866525	1.55953912	-0.95704125

(22)

Ir	0.00000000	0.00000000	0.00000000
C	1.50381025	2.65399139	0.58587629
C	0.79883486	1.31948089	-1.47206625
C	1.81412690	2.30593450	-0.89469852
C	-0.62652577	1.48028224	-1.43049308
C	-1.32113664	2.69986977	-0.80056471
C	-0.69438256	1.47345984	1.36340608
C	-1.63661653	2.47822029	0.70628301
C	0.73399993	1.52227369	1.28299988
C	-0.67427131	-2.81838288	-1.53838215
C	-1.98259349	-2.37250748	-2.18167267
C	-0.16624192	-1.51448269	2.68876721
H	2.80572723	1.83311939	-0.95211962
H	-1.62804978	3.44026642	1.25026083
H	1.28499826	1.04513292	2.09910700
H	2.44127822	2.84390154	1.12666333
H	0.92431504	3.58587503	0.64950981
H	1.87828739	3.22485431	-1.50535650
H	-2.25716347	2.90425018	-1.33898173
H	-0.69906877	3.59753265	-0.93340679
H	-2.65739371	2.08199416	0.80531389
H	1.19889755	0.77332529	-2.33852271
H	-1.19407925	1.01783687	-2.24602281
H	-1.12213984	0.99145130	2.24695488
H	1.17461578	-2.07581545	-0.96868851
H	0.58918224	-1.35135693	-2.33219394
H	-3.42279562	-1.10920516	-1.61806847
H	-2.51800154	-3.26191040	-2.55587456
H	-1.78753387	-1.71182229	-3.04418483
H	-0.86643030	-3.19376626	-0.52690851
H	-0.23267885	-3.62665503	-2.14213003
H	0.13021809	-2.49315909	3.10400037
H	0.48167382	-0.74675993	3.15086665
H	-1.20633741	-1.31580667	3.00958654
N	0.32093229	-1.69393897	-1.39906105

O	-2.77583555	-1.69649293	-1.17498662
O	-0.05386764	-1.56530551	1.26745496

(23)

Ir	0.00000000	0.00000000	0.00000000
C	1.67622867	2.55097924	0.57532388
C	1.06286629	1.11115077	-1.45106922
C	2.11261726	2.02632257	-0.81930553
C	-0.33592286	1.41361304	-1.58935693
C	-0.95351869	2.74647658	-1.13061017
C	-0.68832227	1.63722153	1.17002161
C	-1.44912700	2.67643325	0.34502426
C	0.73399993	1.56485956	1.28299988
C	-1.08953066	-2.82304139	-1.13685040
C	-2.49348102	-2.32654937	-1.50022259
C	0.15244221	-1.42299745	2.78906748
C	-4.32644474	-0.18038691	-1.08622204
H	3.03459484	1.43693509	-0.70672925
H	-1.39013048	3.67062532	0.82391131
H	1.13025662	1.12401580	2.19984077
H	2.56396625	2.70557244	1.20391213
H	1.19226602	3.53402133	0.48596255
H	2.36481970	2.86992403	-1.48945335
H	-1.79515708	3.00787473	-1.78830956
H	-0.22138991	3.55991615	-1.24846378
H	-2.51149001	2.39432271	0.35808303
H	1.49293251	0.46085180	-2.22696041
H	-0.83281790	0.95963163	-2.45602530
H	-1.26395922	1.23871043	2.01300998
H	0.86876990	-2.18667768	-0.93817352
H	0.12291078	-1.54600277	-2.26359239
H	-3.12579169	-3.19056656	-1.74053469
H	-2.47288278	-1.66319945	-2.37482568
H	-1.06197129	-3.17311254	-0.09964944
H	-0.83436569	-3.66522109	-1.80007611
H	0.09991847	-2.44176982	3.21528503
H	1.13042199	-0.99195349	3.08654383
H	-0.64209679	-0.82227164	3.27724288
H	-3.65274991	0.48100750	-1.64407566
H	-4.99619796	-0.72651257	-1.76050929
H	-4.92169120	0.41059586	-0.38256344
N	-0.01838172	-1.76730237	-1.26693921
O	-0.00767618	-1.50814090	1.37192812

S	-3.32083170	-1.39205196	-0.08811580
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(24)

Ru	0.53598795	-0.30693197	0.03268200
C	-2.10123774	-0.79824344	1.18475590
C	-1.04452485	-1.26565897	2.19019159
C	0.12743060	2.00056775	0.25261098
C	-1.14866397	2.40140726	-0.22355041
C	1.12931357	1.58542669	-0.71476507
C	-1.48044826	2.33586676	-1.57020441
C	0.78365774	1.60927294	-2.11625918
C	-0.49748495	1.93838711	-2.51996877
C	1.78788794	-2.94194902	0.59445690
H	-1.95966840	-0.23841473	-0.86013364
H	-1.39021389	-1.79718475	-0.54022829
H	0.41281776	2.22920633	1.27670097
H	-1.87662876	2.79021077	0.48986235
H	-2.46580462	2.65113644	-1.91048444
H	-0.74643032	1.93205924	-3.58077361
H	1.54843741	1.38343336	-2.85839547
H	2.19292144	1.62966141	-0.43548084
H	-2.38597614	0.24126598	1.37943748
H	-3.00261255	-1.42984946	1.18093185
H	-0.87697877	-2.35446397	2.06026811
H	-1.40839789	-1.10429750	3.21996705
H	1.46950087	-3.05135248	1.64637649
H	1.95194949	-3.94944489	0.17408797
H	2.76240159	-2.41434595	0.58500409
N	-1.44075511	-0.82515929	-0.18864294
O	0.16363937	-0.52281794	2.01185242
O	0.80046622	-2.27936398	-0.19815509

(25)-(TS)

Ru	0.66799994	-0.62099994	0.06399999
C	-2.17364434	-0.45542721	1.03279071
C	-1.26339637	-1.10847292	2.07945553
C	0.73758232	1.78141920	0.11936887
C	-0.49649784	2.43998567	-0.11134352
C	1.42719583	1.17214841	-0.99525585
C	-1.09347655	2.44975692	-1.36537441
C	0.79842371	1.22680184	-2.29025408
C	-0.43599996	1.82752059	-2.46199977
C	2.02859086	-2.21023158	0.63184915

H	-1.81429083	0.14745328	-0.95490569
H	-1.73028687	-1.49783693	-0.73880718
H	1.25843674	1.95537633	1.05673893
H	-0.96687962	2.97513479	0.71377427
H	-2.03150062	2.98037376	-1.52355615
H	-0.88782605	1.86410449	-3.45318067
H	1.33223404	0.83142344	-3.15422049
H	2.51113204	1.06405738	-0.95909909
H	-2.26850192	0.61707784	1.23683947
H	-3.17793856	-0.90642339	1.01348336
H	-1.26404920	-2.20749871	1.93406705
H	-1.65307265	-0.90297399	3.09269132
H	2.15306769	-2.31113427	1.72097812
H	2.93115660	-2.47342790	0.05580725
H	2.26176622	-0.73949705	0.59138062
N	-1.49305301	-0.59218849	-0.31307438
O	0.05607762	-0.56711783	2.00173203
O	0.85183307	-2.65597454	0.12174801

(26)-(TS)

Ir	0.00000000	0.00000000	0.00000000
C	1.56395419	2.66060125	0.56592238
C	0.91177353	1.24362969	-1.44937195
C	1.90442477	2.26694537	-0.89426492
C	-0.54460972	1.43414367	-1.45798494
C	-1.21172333	2.71682566	-0.91624825
C	-0.68918322	1.58335395	1.31834691
C	-1.57650948	2.58522719	0.58521717
C	0.73399993	1.58360888	1.28299988
C	-0.87327063	-2.66133543	-1.76186424
C	-1.90817551	-2.00107311	-2.67780028
C	-0.12799713	-1.60937486	1.66854718
H	2.90372240	1.80990747	-0.91992713
H	-1.54162329	3.56693994	1.09123807
H	1.24359034	1.08746588	2.11165554
H	2.49120086	2.82323545	1.13133651
H	1.01955541	3.61541207	0.59408250
H	1.96333257	3.16525488	-1.53668648
H	-2.12293891	2.92482530	-1.49353894
H	-0.54866858	3.57969530	-1.08040991
H	-2.61319331	2.23253456	0.67615332
H	1.31746197	0.71318210	-2.32283959
H	-1.05968848	1.03262857	-2.33685346

H	-1.15590554	1.14667655	2.20395019
H	0.90175648	-2.20910478	-0.73176543
H	0.74433958	-1.41565710	-2.18536697
H	-2.32153907	-0.55759729	-1.38480616
H	-2.50951270	-2.78445093	-3.16000381
H	-1.39275188	-1.44204608	-3.48419283
H	-1.37107580	-3.01875040	-0.85265569
H	-0.42109353	-3.52628286	-2.27441029
H	-0.65879141	-2.57382986	1.55691638
H	-0.36091430	-1.12817499	2.63532459
H	-1.23303676	-0.91016486	0.80533262
N	0.22685501	-1.71608173	-1.34772370
O	-2.84475467	-1.15778634	-1.97777754
O	1.13940412	-1.55743121	1.24084964

(27)-(TS)

Ir	0.00000000	0.00000000	0.00000000
C	1.63916906	2.58258597	0.55888821
C	0.98575724	1.16831654	-1.46947973
C	2.02152443	2.12462746	-0.87506253
C	-0.45615433	1.41997207	-1.48990427
C	-1.07830703	2.74318032	-1.00082703
C	-0.68995721	1.62174700	1.26066894
C	-1.51562575	2.64188465	0.48146651
C	0.73400000	1.56889556	1.28299965
C	-1.05291491	-2.75686485	-1.40968035
C	-1.43989820	-3.21672227	-2.82006122
C	0.06630346	-1.56140124	1.75314302
C	-1.57290728	-0.96956128	-4.72114560
H	2.97905463	1.58565043	-0.83311184
H	-1.47309872	3.62802360	0.97923348
H	1.19669769	1.08913677	2.14894431
H	2.55089364	2.72737924	1.15402308
H	1.14037919	3.56157040	0.52709570
H	2.19218346	3.00071592	-1.52860846
H	-1.94809883	2.99156991	-1.62491634
H	-0.36247787	3.56683897	-1.13993312
H	-2.56500837	2.32013473	0.52778572
H	1.38652248	0.59672699	-2.31896096
H	-1.00036398	0.99193664	-2.33801799
H	-1.20734103	1.22380079	2.13636062
H	0.91514993	-2.12738731	-1.03894712
H	0.21548421	-1.35682631	-2.32797254

H	-1.96014341	-4.17960280	-2.75078747
H	-0.56625929	-3.36748258	-3.46867618
H	-1.93202780	-2.35435731	-0.89988172
H	-0.69053359	-3.61680523	-0.82989141
H	-0.49219546	-2.51809605	1.75101534
H	-0.07782797	-1.00864449	2.70143092
H	-1.12035911	-0.91344356	0.95124270
H	-2.25869944	-0.30273521	-5.25385841
H	-0.99134000	-1.54608626	-5.44791123
H	-0.91880117	-0.35969698	-4.09050237
N	0.03727019	-1.69975529	-1.37633542
O	1.27194328	-1.55926104	1.20477894
S	-2.66998775	-2.09612868	-3.70948841

(28)

Ru	0.37330497	0.61775694	0.33152997
C	2.03873987	-1.84264937	-0.61565574
C	2.74979202	-0.98634747	0.44722543
C	-1.81048341	-1.53871418	0.88784097
C	-2.24212102	-1.60927132	-0.45219930
C	-1.59615022	-0.31127566	1.52768865
C	-2.34367414	-0.43035769	-1.18463693
C	-1.76492245	0.91941854	0.80816940
C	-2.04903781	0.81658724	-0.59237895
C	0.83325753	2.49413034	-0.48085634
H	0.28524104	-1.55363197	-1.75066002
H	1.44650383	-0.37769437	-1.99428344
H	-1.68447085	-2.45732348	1.46072721
H	-2.47493810	-2.57105714	-0.90512099
H	-2.66140679	-0.45768157	-2.22697452
H	-2.20629507	1.72604908	-1.16898141
H	-1.92755196	1.85150073	1.34167605
H	-1.40716980	-0.28612460	2.59814570
H	1.50932688	-2.66867823	-0.12292704
H	2.75711154	-2.26829936	-1.33509563
H	3.38107285	-0.22172686	-0.03869262
H	3.40787631	-1.62347061	1.06460714
H	0.97713010	3.32299411	0.22724686
H	0.18874423	2.73262451	-1.34706497
H	0.39365261	1.55426663	1.60929374
N	1.00773841	-0.98670354	-1.29079067
O	1.79481013	-0.38014752	1.31980640
O	1.86145134	1.65664647	-0.68200189

(29)

Ir	0.00000000	0.00000000	0.00000000
C	1.49891453	2.70495076	0.55456219
C	0.80347790	1.38092794	-1.52110662
C	1.81998410	2.34984670	-0.91931564
C	-0.62281860	1.53012701	-1.43546596
C	-1.31533946	2.74497863	-0.79314027
C	-0.68632143	1.53983810	1.39028200
C	-1.62774858	2.53398411	0.71572919
C	0.73399993	1.58818194	1.28299988
C	-0.79779160	-2.70129256	-1.83650699
C	-1.46191193	-2.47795253	-3.19821631
C	0.57113529	-1.46247225	1.41507397
H	2.80477947	1.86491686	-0.96053815
H	-1.60434640	3.49804392	1.25505343
H	1.29901478	1.09226049	2.07378027
H	2.43390632	2.89905945	1.09728661
H	0.91806381	3.63649720	0.60984304
H	1.90371958	3.26963276	-1.52786706
H	-2.25361015	2.94474659	-1.32838734
H	-0.69390477	3.64146115	-0.93235751
H	-2.64954341	2.14668378	0.82249040
H	1.18324279	0.86341552	-2.41096674
H	-1.19970832	1.07874094	-2.24594619
H	-1.09934240	1.07333392	2.28559712
H	1.01423977	-2.03653754	-0.95678883
H	0.59855943	-1.22817875	-2.32902910
H	-2.11368392	-0.62427599	-3.62789961
H	-1.98661359	-3.40342800	-3.48058408
H	-0.69991870	-2.28541521	-3.97356894
H	-1.55819380	-2.74199503	-1.04926159
H	-0.28061181	-3.67327088	-1.86900988
H	0.17082025	-2.48157514	1.27763722
H	0.54315054	-1.14382632	2.47056365
H	-1.58904981	-0.29624282	0.13974801
N	0.20286723	-1.63049602	-1.46662313
O	-2.45823584	-1.42069251	-3.17313789
O	1.70459482	-1.14081193	0.71257746

(30)

Ir	0.00000000	0.00000000	0.00000000
C	1.43087290	2.74037830	0.51703332
C	0.64786371	1.42121445	-1.54222362

C	1.66714930	2.40968805	-0.98073475
C	-0.77408851	1.52230973	-1.38656906
C	-1.45564154	2.70877431	-0.68380655
C	-0.67379628	1.49732400	1.44758171
C	-1.68158466	2.46653316	0.83575207
C	0.73400000	1.60081431	1.28299965
C	-0.84222180	-2.71011071	-1.71675588
C	-1.29439050	-2.83582047	-3.17681745
C	0.73004075	-1.43493104	1.35870095
C	-1.03953438	-0.33333788	-4.69800056
H	2.65990002	1.95223516	-1.08824754
H	-1.66438044	3.42403956	1.38694761
H	1.35522731	1.10969134	2.03272081
H	2.39887933	2.94384959	0.99398289
H	0.84386102	3.66382916	0.62351969
H	1.69118016	3.34039889	-1.57786974
H	-2.42576515	2.89951886	-1.16270208
H	-0.85995518	3.62030557	-0.83854564
H	-2.68246291	2.04169514	0.98853034
H	1.00693968	0.91810675	-2.44827886
H	-1.38269162	1.05693915	-2.16186818
H	-1.03015539	0.99566575	2.34832760
H	1.05159349	-1.98941882	-1.05018609
H	0.46670260	-1.20665003	-2.37253073
H	-1.94026269	-3.71850254	-3.26369096
H	-0.44120121	-2.99173749	-3.85120212
H	-1.69399454	-2.52341572	-1.05688583
H	-0.39492057	-3.67165675	-1.42314270
H	0.40187871	-2.48052488	1.22989722
H	0.74024984	-1.13584552	2.42051534
H	-1.57213648	-0.35117440	0.20865037
H	-1.52063736	0.63672202	-4.85875200
H	-0.75243048	-0.76359202	-5.66254565
H	-0.15335804	-0.17506554	-4.07600061
N	0.18079736	-1.61527370	-1.47520969
O	1.80744898	-1.03329598	0.59914646
S	-2.32791335	-1.41930495	-3.86424491

(31)

Ir	-0.13799999	-0.50699994	0.69999992
C	1.09662422	-2.02405294	-1.68923032
C	-0.93189215	-0.50965927	-1.28028079
C	-0.31965329	-1.58681369	-2.17052828

C	-0.31086853	0.75533116	-1.01879100
C	1.03256226	1.14938692	-1.65582816
C	1.91659535	-0.39250612	0.18805262
C	2.23645187	0.76946530	-0.75032428
C	1.36399990	-1.65500107	-0.21799998
C	-2.68473459	0.17056685	2.70302207
C	-2.87236055	1.67754600	2.59587863
C	-0.69201147	-4.11488405	1.66078334
C	1.30151977	-1.48050652	3.29394042
H	-0.98920373	-2.45698325	-2.14564754
H	3.12993752	0.55108268	-1.36331493
H	1.59663617	-2.51285210	0.42277024
H	1.17395925	-3.11063103	-1.82995010
H	1.87571774	-1.57664143	-2.32448125
H	-0.27996619	-1.25637493	-3.22397479
H	1.04425325	2.23083860	-1.84971585
H	1.13038475	0.66646178	-2.63968192
H	2.50130836	1.63140632	-0.12107552
H	-2.03019755	-0.53024982	-1.28643123
H	-0.97165770	1.60045745	-0.79872204
H	2.53952709	-0.39882273	1.08599622
H	-2.30020137	-1.51652722	1.53712141
H	-2.89548205	-0.24356372	0.66731471
H	-1.73569064	3.27818445	2.28738065
H	-3.38645685	2.01715222	3.51188203
H	-3.51920601	1.92725273	1.73498759
H	-1.92638719	-0.07499786	3.45501741
H	-3.65083512	-0.25456612	3.02102054
H	-0.76507024	-4.15972971	2.76751324
H	-0.02637442	-4.86207870	1.17718314
H	1.33301902	-2.59018289	3.23567273
H	1.26788427	-1.21436930	4.36531105
H	2.25991383	-1.10204270	2.89564653
N	-2.24640376	-0.48997176	1.42748357
O	-1.58125510	2.32765324	2.47122924
O	-1.28545894	-3.26571987	1.00245908
O	0.15593334	-0.94119857	2.65413108

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Ir	-0.13799999	-0.50699994	0.69999992
C	1.05995789	-2.10911850	-1.66281021
C	-0.98296113	-0.61197371	-1.25752965
C	-0.37383803	-1.71162386	-2.12271347

C	-0.37779155	0.67339630	-1.06846663
C	0.94176756	1.06343112	-1.75617235
C	1.89771093	-0.38644907	0.12462733
C	2.17312435	0.74211042	-0.86642512
C	1.36399990	-1.67435490	-0.21799998
C	-2.59840926	0.28417109	2.77639015
C	-2.82465167	1.79190374	2.64343500
C	-0.71360076	-4.07672026	1.75679412
C	1.38140867	-1.40413111	3.27084161
C	-1.84101484	3.98848999	1.05813528
H	-1.02793275	-2.59046779	-2.05166662
H	3.05664717	0.51342315	-1.48968445
H	1.62793626	-2.50067408	0.45127472
H	1.15777630	-3.19889524	-1.75735749
H	1.81694181	-1.68023439	-2.33683543
H	-0.36570073	-1.41846535	-3.18769761
H	0.92889394	2.13583684	-1.99459752
H	1.02367672	0.54191419	-2.72140841
H	2.43689055	1.63216859	-0.27726339
H	-2.07989229	-0.65656006	-1.22635111
H	-1.04847568	1.51597177	-0.87178385
H	2.53699491	-0.33686390	1.00974743
H	-2.24020344	-1.42645875	1.67012599
H	-2.89236121	-0.19670970	0.76709916
H	-3.30224388	2.14586216	3.56486417
H	-3.50100295	2.01410047	1.80611532
H	-1.81676328	0.03949612	3.50343535
H	-3.55142561	-0.13811870	3.13872723
H	-0.68038897	-4.09762904	2.86516285
H	-0.10391992	-4.84186661	1.22764798
H	1.40874077	-2.51290765	3.20711007
H	1.38163833	-1.14078720	4.34327927
H	2.32616678	-1.02276471	2.84402396
H	-2.50882006	4.76126952	1.45247949
H	-0.94625387	4.46215414	0.63957393
H	-2.34070800	3.43577857	0.25532984
N	-2.20509999	-0.40417526	1.50486222
O	-1.35845367	-3.23295262	1.14137118
O	0.21610452	-0.85926531	2.66902335
S	-1.25901533	2.82224049	2.38847314
(33)-(TS)			
Ir	-0.13799999	-0.50699994	0.69999992

C	1.33274573	-1.75423320	-1.75802884
C	-0.57932941	-0.15192980	-1.32147755
C	0.03923057	-1.12205863	-2.32580731
C	0.11729001	0.98929920	-0.73795544
C	1.58334169	1.32217463	-1.07896767
C	1.97824872	-0.63873779	0.52039033
C	2.57089793	0.62508289	-0.10284258
C	1.36399990	-1.70118898	-0.21799998
C	-2.88841740	0.55071798	2.23867600
C	-3.07743998	2.04220892	1.97613689
C	0.25676189	-2.58887748	3.14667769
C	0.95770340	-0.15173037	3.70537578
H	-0.69541192	-1.91469715	-2.52913460
H	3.53006162	0.40641041	-0.60662448
H	1.35618933	-2.68347755	0.26285762
H	1.42503066	-2.80245037	-2.07318765
H	2.21661796	-1.24187148	-2.16414456
H	0.23612696	-0.62536523	-3.29318264
H	1.73068703	2.40973947	-1.03274465
H	1.80050884	1.03273096	-2.11854530
H	2.80696640	1.31544614	0.71944491
H	-1.65169681	0.00740440	-1.51099732
H	-0.49268439	1.87153906	-0.51549088
H	2.44014487	-0.91296141	1.47321138
H	-2.49354536	-1.21780999	1.23338298
H	-2.77327990	0.04869891	0.20958458
H	-1.94896010	3.65901338	1.71569418
H	-3.74721269	2.44126651	2.75683319
H	-3.58216906	2.19715020	1.00475116
H	-2.23671759	0.37632727	3.10002120
H	-3.88328331	0.13233005	2.45853266
H	-0.11924360	-3.04160989	4.08581868
H	1.19338655	-3.06130756	2.77887097
H	0.84741179	-1.50055765	3.68659412
H	0.74319572	0.01389924	4.77994336
H	2.04152982	-0.08556836	3.46895520
N	-2.29373061	-0.21865048	1.08166483
O	-1.80172693	2.73363981	2.00515009
O	-0.62776062	-2.17222700	2.28270317
O	0.09356882	0.31520461	2.86426865
(34)-(TS)			
Ir	-0.13799999	-0.50699994	0.69999992

C	1.16875453	-1.96834091	-1.72303412
C	-0.78604510	-0.41292229	-1.27912097
C	-0.23152403	-1.50033967	-2.19722742
C	-0.08931851	0.82113303	-0.92586882
C	1.31263503	1.16775565	-1.46013939
C	1.96751554	-0.55039709	0.31761286
C	2.42686298	0.64574244	-0.51376428
C	1.36399990	-1.72633801	-0.21799998
C	-2.50354620	0.99870057	2.42466209
C	-2.82233495	2.40582820	1.90604086
C	0.25837159	-2.86322022	2.90954122
C	1.15928308	-0.55710246	3.66357964
C	-2.07165717	5.01997749	1.02033005
H	-0.93168283	-2.34780789	-2.16421123
H	3.34014497	0.39520987	-1.08370510
H	1.46719078	-2.64373184	0.36608883
H	1.29487459	-3.03700047	-1.94500589
H	1.95808271	-1.45027980	-2.28679720
H	-0.20063579	-1.16979784	-3.25113408
H	1.40216556	2.25770167	-1.56249872
H	1.44509428	0.75851334	-2.47315175
H	2.70890780	1.44612873	0.18419259
H	-1.88010662	-0.32661241	-1.37256180
H	-0.71095356	1.70640905	-0.76163095
H	2.50932051	-0.66537210	1.26024292
H	-2.41809137	-0.93599484	1.68730298
H	-2.77946964	0.17983682	0.51690547
H	-3.44593809	2.92341407	2.64562360
H	-3.38264692	2.37328016	0.96004820
H	-1.64926634	1.01061242	3.10871811
H	-3.38172043	0.61992045	2.96842088
H	-0.08737509	-3.40648819	3.81067294
H	1.11681826	-3.35257799	2.40168980
H	0.95436365	-1.88810713	3.53691693
H	1.05824174	-0.48413365	4.76438006
H	2.21483727	-0.54691066	3.31949810
H	-2.74953778	5.44129089	1.77174712
H	-1.25256014	5.72612328	0.84850317
H	-2.60788407	4.83435496	0.08270664
N	-2.17367077	0.00197429	1.33075298
O	-0.65680998	-2.28258579	2.18906691
O	0.25460755	0.03669314	2.94850135
S	-1.27753961	3.45513260	1.65532470

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Ir	-0.13799999	-0.50699994	0.69999992
C	1.26473601	-1.75523939	-1.75343289
C	-0.57410610	-0.03328792	-1.32196644
C	-0.04419421	-1.10096890	-2.27592010
C	0.18684751	1.04291052	-0.75929580
C	1.66558925	1.29347322	-1.08719012
C	1.97456232	-0.66551244	0.52945635
C	2.59693306	0.59748972	-0.05987429
C	1.36399990	-1.71844936	-0.21799998
C	-2.59154138	0.94802294	2.41054462
C	-2.57143355	2.45126624	2.14026359
C	0.61955270	-2.27791516	3.09612715
C	1.81194330	0.79701359	4.33901215
H	-0.82072693	-1.87659302	-2.35470589
H	3.58345418	0.37978280	-0.50924606
H	1.34328822	-2.70478849	0.25300291
H	1.30563079	-2.80378843	-2.07986276
H	2.13522435	-1.25825987	-2.20254439
H	0.10156498	-0.70596444	-3.29735109
H	1.86378412	2.37398221	-1.08324571
H	1.89282628	0.94844624	-2.10623961
H	2.77879885	1.29056419	0.77352743
H	-1.64780006	0.15767571	-1.46654719
H	-0.36343148	1.94580660	-0.47840434
H	2.39804143	-0.94223953	1.49962368
H	-2.52933132	-0.86781005	1.42510616
H	-2.68625529	0.41991356	0.38966651
H	-1.26315102	3.93062768	1.93834285
H	-3.19317202	2.93375431	2.91445850
H	-3.04648197	2.65667144	1.16051729
H	-1.94808742	0.66792183	3.24966896
H	-3.63397682	0.69921075	2.66676130
H	0.15838639	-2.96632556	3.82467240
H	1.25692077	-2.87823415	2.41941681
H	1.30489170	-1.61884021	3.67299737
H	1.57217617	0.42097485	5.36400007
H	2.87623577	0.67877548	4.02227823
N	-2.19013389	0.08601148	1.23060948
O	-1.22648438	2.98390651	2.19072392
O	-0.38417880	-1.52609551	2.43864471
O	0.97136294	1.31448997	3.62046689

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Ir	-0.13799999	-0.50699994	0.69999992
C	1.31430483	-1.77613365	-1.75239925
C	-0.51919655	-0.04317833	-1.33891327
C	0.01583741	-1.11164239	-2.28936284
C	0.25742074	1.01845870	-0.76804175
C	1.74872038	1.24365949	-1.06442086
C	1.97933800	-0.71783380	0.55381121
C	2.64744477	0.52560415	-0.02254053
C	1.36399990	-1.74855984	-0.21799998
C	-2.53786215	1.03581450	2.42689152
C	-2.45859130	2.54053124	2.13770394
C	0.55214511	-2.32320180	3.07925331
C	1.64415989	0.59406110	4.88648704
C	-0.92516363	4.54233715	0.79405447
H	-0.76212892	-1.88196952	-2.39484645
H	3.63038508	0.27007956	-0.45974217
H	1.32552727	-2.73868853	0.24413464
H	1.35872915	-2.81627520	-2.10186646
H	2.19863224	-1.27343621	-2.16814605
H	0.17898877	-0.69869874	-3.30131737
H	1.96144598	2.32148489	-1.04742387
H	1.99186781	0.90580153	-2.08217949
H	2.84779733	1.21034321	0.81306505
H	-1.58370265	0.17125500	-1.51479547
H	-0.27039254	1.94056368	-0.51544776
H	2.37975233	-1.01325803	1.52811246
H	-2.52449811	-0.79109072	1.46572288
H	-2.66132610	0.48455016	0.41785093
H	-3.05308203	3.05916536	2.89854282
H	-2.88954819	2.77299240	1.15213606
H	-1.90065043	0.74798846	3.27057236
H	-3.57973541	0.79938427	2.69740915
H	0.05542992	-3.01597156	3.78019645
H	1.14803046	-2.93065291	2.37445888
H	1.27412599	-1.72079140	3.67147387
H	1.17614562	0.06074174	5.74387203
H	2.73360636	0.41143088	4.73475700
H	-1.65506256	5.32458598	1.02998229
H	0.05331660	5.00786117	0.63868677
H	-1.21366498	4.02408295	-0.12907714
N	-2.16190749	0.15066274	1.25525407
O	-0.41450903	-1.49406150	2.45231850

O	1.00968067	1.33679714	4.16193627
S	-0.73329689	3.30999754	2.18207646